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EPR of trivalent iron ions in a LiCaAlF6 crystal

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Abstract

The orientational dependences of the EPR spectra of Fe3+-doped LiCaAlF6 single crystals (space group P31c, Z=2), grown at the Laboratory of Magnetic Radio Spectroscopy at Kazan' State University, have been investigated in detail. The spectrum is described by a trigonal spin Hamiltonian with the following parameters: B20=40.072 × 10-4 cm-1, B40= - 5.799 × 10-4 cm-1, B43= - 4.281 × 10-4 cm-1, As = 24.33 ± 1, Ap = 6.13 ± 1, g∥ = g⊥ = 2.00217 ± 0.0003. A theoretical calculation of the hyperfine structure parameters shows that they are described quite well when allowance is made for the overlapping of the wave functions of the paramagnetic center and the ligands (F-).